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13. ABSTRACT *(Maximum 200 Words)*

Calculations were performed of the formation energies of transition metal carbides and silicides in order to evaluate the thermodynamic limitations to incorporation of these elements as dopants in Silicon carbide. The prospects of SiC as a host for dilute magnetic semiconductor applications by doping with Cr and Mn were evaluated. Calculations were performed for MnN and Mn3N2 compounds and a model developed for explaining their antiferromagnetic order in terms of exchange interactions between near neighbors. Densities of states calculations of these materials were used to interpret spin-polarized scanning tunneling microscopy data.

Calculations were performed for FeN in zincblende and rocksalt structure to compare their relative stability and magnetic properties. Calculations of the preference for ferro or antiferromagnetic coupling were performed for GdN. Program development work on magneto-optics and methods beyond LDA was initiated.

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Performance Report

Magneto-Optical Properties of Hybrid Magnetic Material Semiconductor Nanostructures

Grant No.: N00014-02-1-0880
Period of Performance: July 15, 2002- August 31, 2003

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1 Objectives

The objectives of the grant are to develop computational approaches for magneto-optical properties based on first-principles density functional calculations including effects beyond the local density approximation and to apply them to systems of interest to the emerging field of spintronics. These magneto-optical properties provide a possible link between theory and experimental characterization efforts and are of interest for device applications in their own right.

Systems of interest include epitaxial heterojunctions between magnetic compounds compatible with semiconductors, magnetic semiconductors and other nanoscale hybrid quantum well systems.

2 Status of effort and Accomplishements

2.1 Personnel and Expenditures

The progress was delayed by the difficulty of obtaining personnel in the start-up period. A student who was targetted originally to work on the project left our department in August 2002. New students became availabe to the project only in May 2003. One graduate student (Pavel Lukashev) received initial training in the methodologies to be used in the project during the period January-May without being supported on the project and joined the effort in May 2003. Identifying a postdoc for the project also was a time consuming process. A person was identified in March 2003 and he joined the effort on August 2003. His name is Paul Larson. He was formerly at the Naval Research Laboratory.

Due to this lack of personnel, the expenditures during the first year were minimal, including only summer salary of the PI for 2002 and summer 2003, salary support for a graduate student from May 2003-August 2003, i.e. only 4 summer months during which time only stipend has been spent, no tuition costs, and one month of a postdoctoral research associate. A small amount was also spent on updating computing equipment and on travel to a conference in July 2002 and the APS March Meeting 2003.

Fortunately, these start-up problems have now been resolved. The group is fully operational and further enhanced by a related effort supported by NSF which also employs another graduate student who started end of August.

2.2 Technical Progress

Nevertheless some noteworthy technical progress was made during the first year. Although it has primarily consisted in finishing on-going projects which were initiated prior to the start of this grant, some new efforts were started.

One of the projects is a continuation of an earlier ONR grant on the properties of Transition Metal Doped Silicon Carbide. The prospects of this system as a dilute ferromagnetic semiconductor host were investigated. As part of finishing up the write-up of a final publication on this work, some additional calculations were found necessary. These included full-potential calculations on a few test cases to check the initial results which had been obtained using a more approximate atomic sphere approximation method. Furthermore the energies of formation of several transition metal carbides and silicides were calculated and their basic magnetic properties examined in order to analyze the thermodynamic aspects of the feasibility of transition metal doping in SiC. These calculations and their relevance to the problem are presented in Phys. Rev. B **68**, 125204 (2003), a copy of which was already sent to the program manager.

A second system which was investigated is that of manganese nitride compounds: MnN and Mn_3N_2. These materials are of interest as possible contaminating phases in Mn doping of GaN and as possible magnetic metallic compounds to make heterojunctions with GaN. Our study of these compounds was mostly motivated by the recent experimental work of Arthur Smith at Ohio University (Athens, Ohio) who is growing these materials as thin films by MBE on MgO substrates and has included Spin-Polarized Scanning Tunneling Microscopy (SP-STM) investigations. Our efforts supported under the grant consisted of a collaboration with Arthur Smith to analyze the SP-STM and of calculations of the magnetic interactions and the formulation of a Heisenberg type model that can explain the basic magnetic ordering tendencies in these materials based on our earlier calculations of the electronic structure. The collaboration with Art Smith led to two publications so far, one of them in Phys. Rev. Lett. **89**, 226101 (2002), the other one submitted to Surf. Sci. The PRL has received considerable attention— for instance it was mentioned in the News section of the MRS Bulletin — because it constitutes one of the first demonstrations of SP-STM with atomic resolution displaying magnetic and chemical ordering simultaneously. Our main work on the electronic structure of these materials and how they affect the magnetic properties and ordering was written up during summer 2003 and was meanwhile accepted for publication in Phys. Rev. B.

A postdoctoral research (Maosheng Miao) associate contributed substantially to both these "continuation of earlier efforts" projects and was part time supported on the grant.

An initial project was assigned to the graduate student Pavel Lukashev to learn electronic structure calculations of magnetic materials. This project concerns a continuation of our interests in the properties of transition metal nitrides and dealt with FeN. This material has been proposed to have zincblende rather than the usual rocksalt structure which may be highly beneficial for forming heterojunctions with semiconductors. Our calculations support these experimental claims but show the material to be magnetic only in the rocksalt phase, not in the zincblende phase. Experimental indications of magnetism in this system must thus be attributed to impurity phases. This work will be presented at a poster session at the Ohio Sectional Meeting of the APS in October 2003.

Work was also initiated by our new postdoc (Paul Larson) on implementing the LDA+U method in our codes. This will be a starting point for a new Screened Exchange method whose extension to open shell systems will resemble the LDA+U approach but with a first-principles approach to calculating the U's. As a test system for this work, we will use GdN which is an interesting bulk ferromagnetic semiconductor with magnetism due to the half-filled open 4f shell. To establish a baseline, Local spin density calculations were performed first. These calculations confirm the ferromagnetic rather than antiferromagnetic order in this material and a first analysis of the exchange interactions is in progress.

3 Personnel Supported

- PI Walter Lambrecht, one month summer salary during 2002 and one month salary during 2003.
- Postdoctoral Research Associate Paul Larson, full time supported on this grant as of August 2003.
- Senior Research Associate, Maosheng Miao, part time supported on the grant during summer 2003.
- Graduate student research assistant, Pavel Lukashev, full time supported on the grant as of May 2003.

4 Publications

- Magnetic properties of substitutional 3d transition metal impurities in silicon carbide, M. S. Miao and W. R. L. Lambrecht Phys. Rev. B **68**, 125204 (2003)
- Atomic-Scale Spin-Polarized Scanning Tunneling Microscopy Applied to Mn3N2(010), H. Yang, A. R. Smith, M. Prikhodko, and W. R. L. Lambrecht, Phys. Rev. Lett. **89**, 226101 (2002)
- Electronic structure and magnetic interactions in MnN and Mn_3N_2, Walter R. L. Lambrecht, Margarita Prikhodko, and M. S. Miao, accepted for publication in Phys. Rev. B (2003).
- Atomic-Scale Structure of η-phase Mn3N2 (010) Studied by in-Situ Scanning Tunneling Microscopy and First-Principles Theory, Haiqiang Yang, Rong Yang, Arthur R. Smith, and Walter R. L. Lambrecht submitted to Surface Science

5 Interactions/Transitions

Collaborations: collaboration with Arthur Smith, Ohio University, Athens Ohio.

Presentations at conferences:

- Magnetic Properties of Transition Metal Impurities in SiC, M. S. Miao and Walter R. L. Lambrecht, invited talk at ESCM 2002, Electronic Structure and Computational Magnetism, 15-17 july 2002, Georgetown University, Washington, DC
- Magnetic Properties of Mn-N Compounds, Margarita Prikhodko and Walter R. L. Lambrecht, contributed poster at ESCM 2002, Electronic Structure and Computational Magnetism, 15-17 july 2002, Georgetown University, Washington, DC
- Electronic structure and magnetism in MnN compounds, Margarita Prikhodko and Walter R. L. Lambrecht, contributed talk at Symposium P, Novel Aspects of Spintronic Materials and Devices, Mater. Res. Society (MRS) Fall Meeting in Boston, December 2-5, 2002.
- Atomic-scale Spin-polarized Scanning Tunneling Microscopy studies of the surface magnetic structure of Mn_3N_2 (010), Haiqiang Yang,

Arthur R. Smith, Margarita Prikhodko, Walter R.L. Lambrecht Bull. Am. Phys. Soc. **48** N14.009 (2003)

- Bias-Voltage-Dependent Magnetic Contrast in Spin-Polarized Scanning Tunneling Microscopy Rong Yang, Haiqiang Yang, Arthur R. Smith, Margarita Prikhodko, Walter R.L. Lambrecht, Bull. Am. Phys. Soc. **48** N14.010 (2003).

- New Materials for Spintronics and Nonlinear Optics, M. S. Miao, X. Jiang and Walter R. L. Lambrecht, Research Showcase 2003, Case Western Reserve University, Cleveland, OH April 4 2003.

- First-principles study of CoN and FeN, Pavel Lukashev and Walter R. L. Lambrecht, Fall Meeting of the Ohio Section of the APS, October 17-18, 2003 Case Western Reserve University, Cleveland, Ohio

6 Honors/Awards

The PI became a Fellow of the American Physical Society, 2003.